1,4-Dimethyl-3-aminocarbazole

111249-52-6 | DTXSID80149567

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 2200 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.01e-01

Confidence level: 6.57e-01

Nearest Neighbors from the Training Set

Image not found

9-Anthracenecarboxylic acid
Measured: 550
Predicted: 1400

Image not found

9-Anthracenemethanol
Measured: 4070
Predicted: 5400

Image not found

2-Acetylaminofluorene
Measured: 1380
Predicted: 1860

Image not found

Anthraquinone
Measured: 3720
Predicted: 2300

Image not found

2-Aminoanthracene
Measured: 28200
Predicted: 24300